2-Methoxyethyl acetate

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Model Performance

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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 3.14 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.03e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

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2-Methoxyethyl acetate

Measured: 8.46 Predicted: 3.14

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Methyl 3-methoxypropionate

Measured: 6.35 Predicted: 3.06

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1-cyanoethyl acetate Measured: 1.77 Predicted: 1.78

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Ethyl cyanoacetate Measured: 1.77e-01 Predicted: 9.98e-01

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Methyl 3-ethoxypropanoate

Measured: 8.47e-01

Predicted: 1.24